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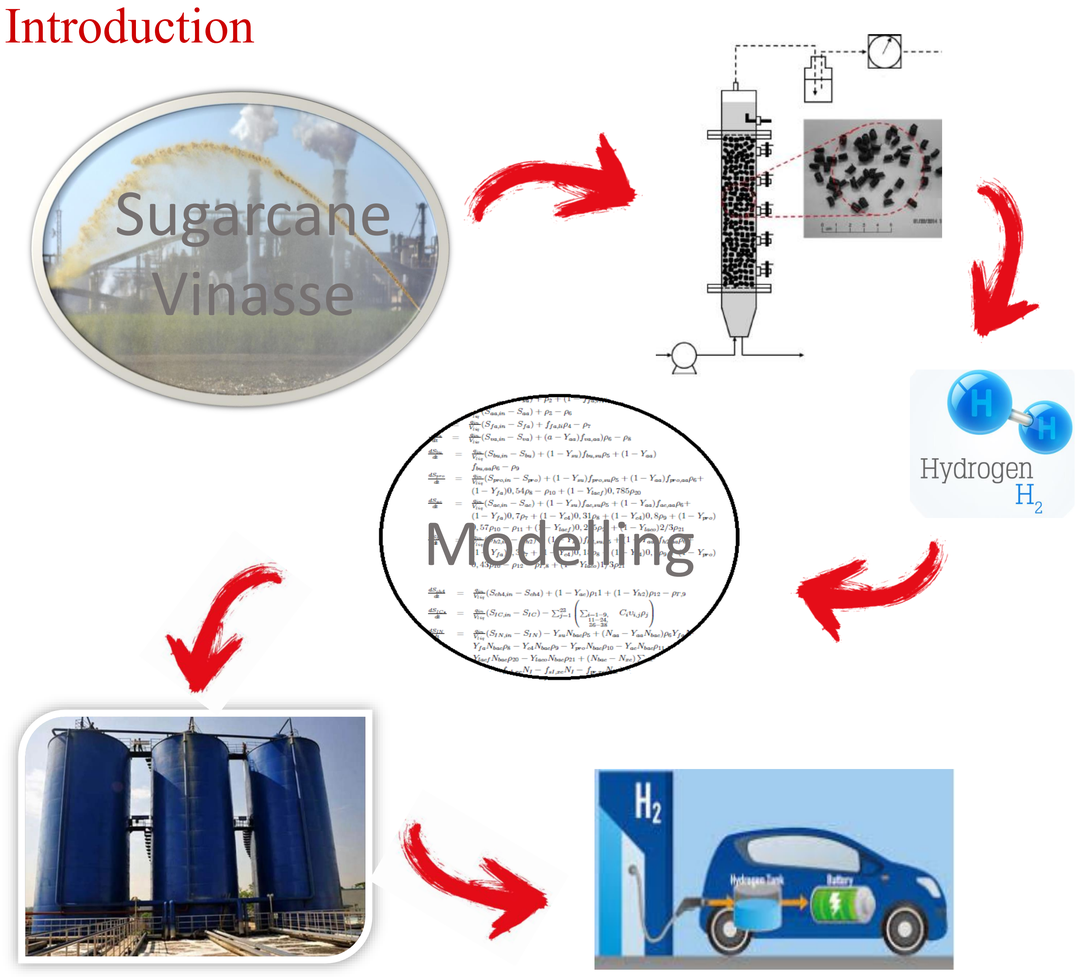
Modelling of an Anaerobic Packed Bed Reactor used in processing of sugarcane vinasse to recover hydrogen using the Anaerobic Digestion Model Number 1

Couto, P. T [a,b].; Fuess L. T. [a] ; Nopens, I. [b]; Zaiat, M. [a] ; Ribeiro R. [c]

[a] Biological Processes Laboratory, School of Engineering of São Carlos (EESC), University of São Paulo, São Carlos/SP, Brazil
[b] Department of Mathematical Modeling, Statistics and Bioinformatics (BIOMATH), Ghent University, Ghent, Belgium
[c] Faculty of Animal Science and Food Engineering (FZEA), University of São Paulo (USP), Pirassununga/SP, Brazil

1. Introduction



2. Objective

Apply ADM1 to model the processing of sugarcane vinasse in an Anaerobic Packed-Bed Reactor (APBR) to simulate:

- The recovery of hydrogen;
- Consumption and production of volatile fatty acids;
- Removal of carbohydrates.

3. Methodology

Experimental phase:

- Acidogenic packed bed reactor (APBR) operated by Fuess et. al. (2015);
- Condition: thermophilic (55°C);
- Volume: 2.3 L;
- Operation time:240 days;

Modelling phase:

- Data from day 206 selected: Considerable H2 production and constant operational conditions;
- First hypothesis assumed to modeling:

Hypothesis 0: ADM1 - Methanogenesis pathways = ?

- Assumptions: degraders Xac and Xh2 removed in ADM1; Sch4 = 0;
- Direct validation of model with experimental data performed;
- If hypothesis 0 fails to describe data, alternative hypothesis is assumed:

Hypothesis 1: ADM1 – Methanogenesis + Lactato pathways = ?

- Proposed ADM1 modifications:
  1. Production of lactate from sugar:

$$C_6H_{12}O_6 \rightarrow 2CH_3CHOHCOOH$$

  2. Production of butyric acid from acetic acid and lactic acid:

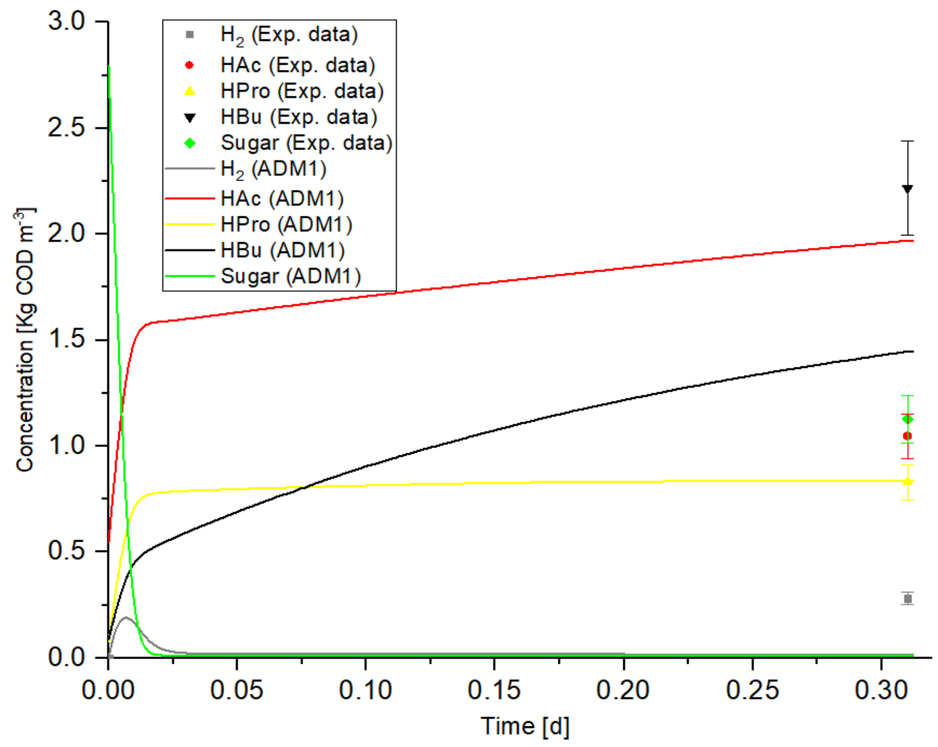
$$CH_3COOH + 2CH_3CH(OH)COOH \rightarrow H_2 + 3/2CH_3(CH_2)_2COOH + 2CO_2 + H_2O$$

  3. Production of butyric acid from lactic acid:

$$3CH_3CH(OH)COOH \rightarrow 2CH_3CH_2COOH + 2CH_3COOH + CO_2 + H_2O$$

- Direct validation of the model with experimental data;

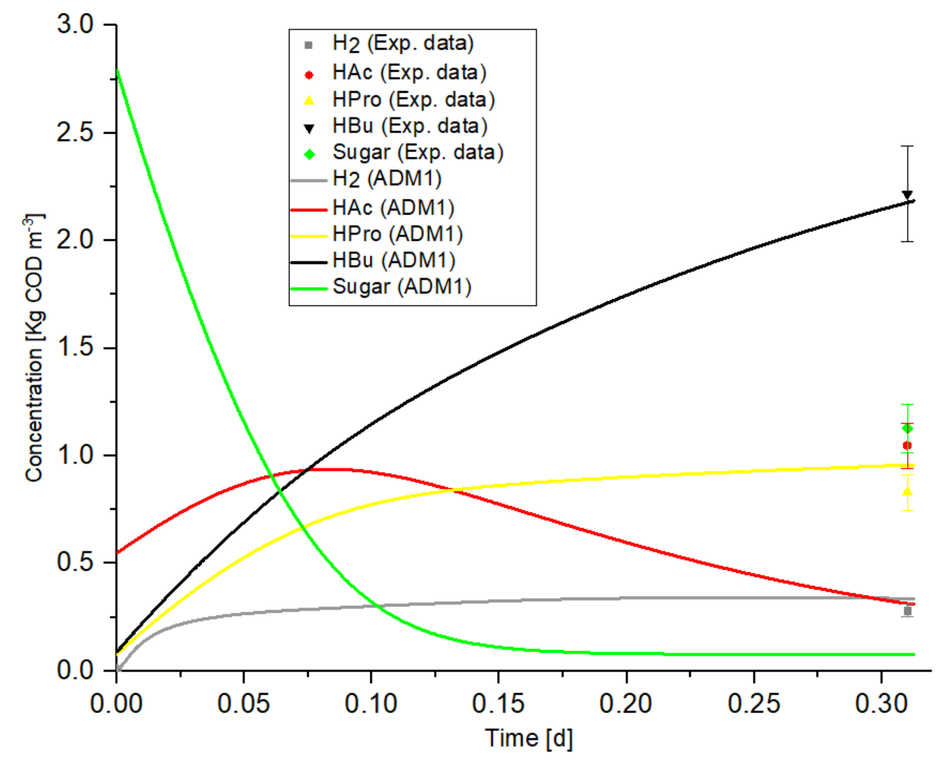
4. Results and Discussion



Hypothesis 0 accepted?

NO

- Overprediction of acetic acid; Underprediction of butyric acid;



Hypothesis 1 accepted?

YES

- Good prediction of butyrate; still underprediction of acetate;
- Hypothesis 1 is better;
- However, further improvements in the model are required.

5. Conclusions

- Modified ADM1 predicts behaviour of APBR better -> production of butyrate from acetate and lactate needed to be included;
- Batch Experimental tests are required to determine the Yields coefficients -> f_bu_ac and f_bu_lac.

6. Acknowledgments

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7. References

FUESS, L. T. et al. (2015) **Operational strategies for long-term biohydrogen production from sugarcane stillage in a continuous acidogenic packed-bed reactor**. International Journal of Hydrogen Energy, v. 41, n. 19, p. 8132–8145.

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